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The Superperiod of the Nonlinear Weighted String (FPU) Problem*

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This paper gives some history of the problem, and includes superperiod data for quadratic and cubic nonlinear terms, together with a computation for a prime number of particles in the string. Extension of the problem to a circular array is discussed, and there is a bibliography.

The Maniac I computer (N. Metropolis) started working at Los Alamos early in 1952. E. Fermi, who was visiting the Laboratory, J. R. Pasta, and S. M. Ulam entertained themselves by considering what new problems it opened up for study. One such, in classical fluid theory in its simplest approximation [1], considers a linear array of atoms linked by nonlinear forces. The results of the first calculations, which were coded by one of us (M.T.M.), were so surprising that the investigators were enticed into a study of nonlinear systems generally. The first system to be examined (Fig. 1) consisted of a one-dimensional array of mass points linked by light Hookean springs—tension $\propto$ extension—made nonlinear by addition of a small term α (extension) [2] or β (extension) [3].

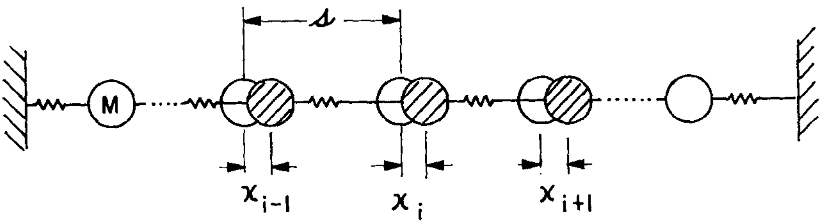

FIGURE 1

* Work performed under the auspices of the U. S. Atomic Energy Commission.

Thus:

$$\begin{aligned}\text{force } F_i \text{ on } i\text{th particle} &= (K/s)[(x_{i+1} - x_i) - (x_i - x_{i-1}) \\ &\quad + \alpha(x_{i+1} - x_1)^2 - \alpha(x_i - x_{i-1})^2 \\ &\quad + \beta(x_{i+1} - x_i)^3 - \beta(x_i - x_{i-1})^3]\end{aligned}$$

(K = Hookes'constant of elasticity).
From Newton:

$$\partial^2 x_i/\partial t^2 = F_i/M = K/Ms\,[\ldots]. \tag{1}$$

By analogy with the wave equation

$$\partial^2 x/\partial t^2 = c^2(\partial^2 x/\partial s^2),$$

the propagation velocity

$$c = \sqrt{Ks/M},$$

while the time period of the fundamental frequency, for a chain of N masses:

$$\tau = 2 \times \frac{\text{length}}{\text{velocity}} = 2Ns\sqrt{M/Ks} = 2N\sqrt{Ms/K}.$$

Setting $M = s = K = 1$ for the computation,

$$\tau = 2N.$$

As Fermi observed, nobody at that time could state, without calculating it out first, what such a string, started out with a pure sinusoidal displacement, would look like after a few thousand ocsillations at its fundamental frequency, although statistical mechanics makes general statements about the diffussion of energy and equipartition among modes, and Poincaré tells us [2] that all accessible points in phase space will be approached arbitrarily closely.

At $t = 0$, the x_i were given some selected configuration (usually half sinusoid), and using Eq. (1), the computer computes the new x_i's one time step δt ahead and so on. The number of points chosen was 64 or 32 (which symmetry allows to be halved in some cases), the ends of the string were fixed, and the amplitude of the starting half sinusoid, together with the nonlinear coefficient α or β, chosen to give a ratio of nonlinear to linear term of no more than 10%. Initially, this occurs at the fixed ends of the string, where it is most stretched. In the first FPU problem, $N = 16$, the displacement sin $\pi i/16$, the time step $\delta t = 1/8$, the quadratic term $\alpha = 1/4$. Hence from Eq. (2), the time period of the first mode (fundamental) $\tau = 32$; and the ratio $\tau/\delta t = 32/^{1/8} = 256$. In our discussion, we measure time (abcissae) in units of τ. The FPU paper measured time in cycles, meaning computational cycles—δt.

At first the problem behaved as expected and energy appeared and grew in harmonics of the fundamental, but soon the process became strangely selective and not diffusion-like. At 25 oscillations, the string configuration began to retrace its steps, passing through previous complications in reverse order. By $\sim$50 oscillations, the complications were unscrambled and the string was back—all but a discrepancy of a few percent—to its half sinusoid starting configuration (Fig. 2, upper). Other force laws, cubic and discontinuous, showed complications differing in detail but with similar recurrences (Fig. 4, upper). This behavior was not at all according to statistical-mechanical expectations. Nor was it Poincaré-like; for example, the time for the recurrence of N particles to $1 - \epsilon$ of their starting configuration is given [3] by $\tau_{\text{poin}}/\tau = (2\pi)^{N-2}\,\epsilon^{2-N}\,N^{-1}$. For $N = 16$, $\epsilon = 1/100$, this amounts to 10^{35} oscillations! Fermi became quite excited and thought that something new and important might be at hand. This happened in 1953; Fermi's untimely death occurred in November 1954. In the following year, J. Pasta, who had left the laboratory, returned to make a few more computer runs and assemble the material which appeared as Los Alamos Report LA-1940 (Physics) dated November 2, 1955 [4].

This attracted the attention that might have been expected for such a quiet publication in a noisy world. Few, if any, references to it appeared in the literature over the next 5 years, but the results circulated as a piece of mathematical curiosa by word of mouth.

One of us (J.L.T.), who had been an interested bystander to these events was nagged by the existence of what seemed to be loose ends to the FPU problem but was too involved elsewhere (controlled fusion) to do anything. For example, the few percent closing error at recurrence was one of these. Such a magnitude seemed incongruous—it should either be much more, or essentially zero. Might it really be zero, concealed by a computer roundoff error or noise? If not, could it be that the few percent was the real manifestation of equipartition, the rest being excursions produced by transient subharmonic resonances between modes?

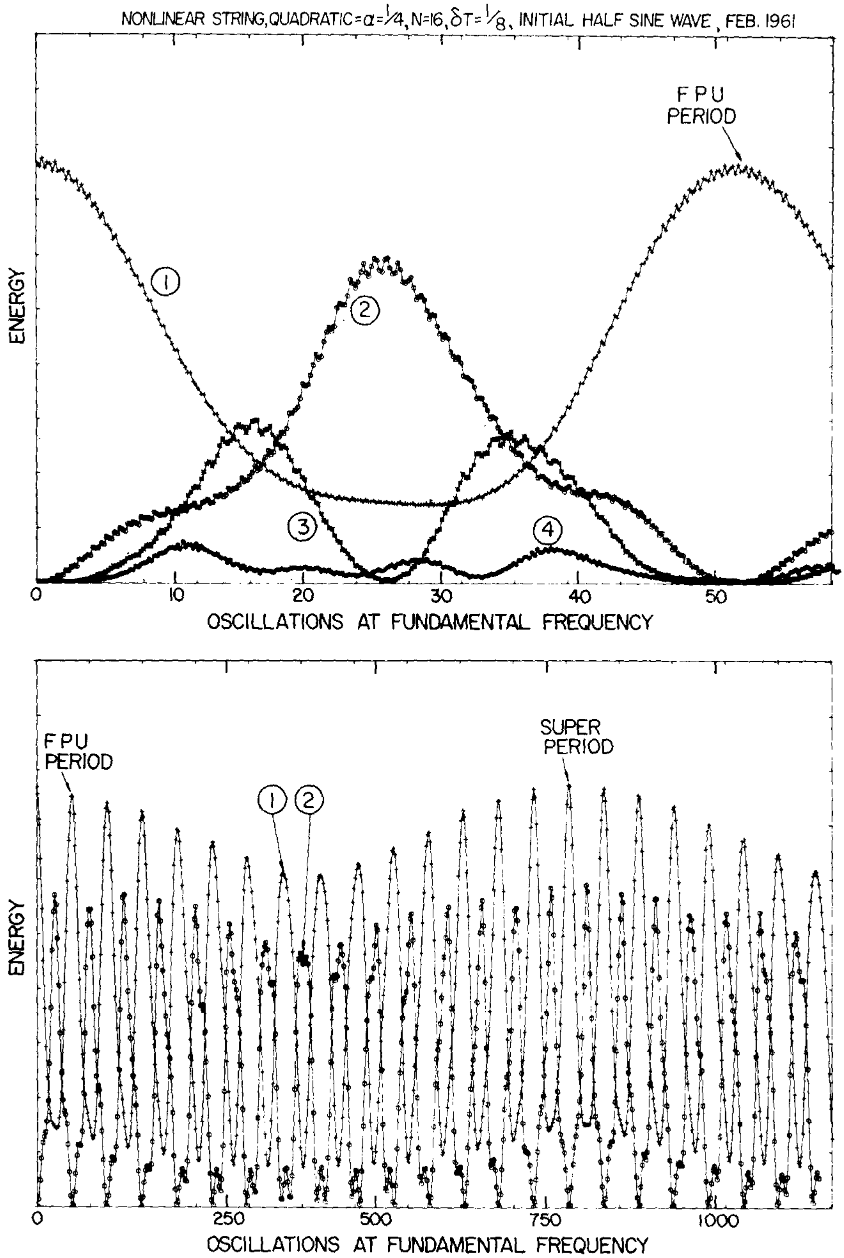

FIG. 2. The upper figure recalculates the Fermi-Pasta-Ulam[4] result,

$$\ddot{x} = (x_{i+1} - x_i) - (x_i - x_{i-1}) + \alpha[(x_{i+1} - x_i)^2 - (x_i - x_{i-1})^2]$$

$i = 1, \ldots, N$, $N = 16$, $\alpha = 0.25$, (1) = 1st Mode (Fundamental), (2) = 2nd Mode, etc. The ordinates are the total energies calculated from

$$E = E^{\mathrm{kin}} + E^{\mathrm{pot}} = \tfrac{1}{2}\dot{a}_k^2 + \tfrac{1}{2}a_k^2 \sin^2 \frac{\pi k}{2N}; \qquad a_k = \sum_i x_i \sin \frac{ik\pi}{2N}$$

Fundamental period	τ	$256\ \delta t =$	32		
FPU period	τ'	$13{,}231\ \delta t =$	165	$= 51.95\ \tau$	
Super period	$\tau'' =$	$200{,}647\ \delta t =$	2508	$= 783.7\ \tau$	$= 15.2\ \tau'$

In early 1961, for one of us (J.L.T.) some healthy participation in science for its own sake became an urgent need, and FPU provided this. The first task was to repeat the original FPU results and this; after some false starts, we were able to do (Fig. 2, upper). Ordinates are the energy computed in the numbered harmonic. To test for the trivial (noise) explanation, at the first recurrence, the computer was set to retrace its 13 000 time steps. It did so, recovering the initial configuration to within 8 decimal places. Hence the trivial explanation could be dismissed.

This out of the way, we proceeded to run the problem forward. Obviously, if the conjecture about equipartition was correct, the closing error should mount at each recurrence until it became random. At the next recurrence, the closing error was doubled, and it continued to increase, levelling off at about 390 fundamental oscillations to an amplitude 20% below the starting amplitude. At the next recurrence, our complacency was jolted, the closing error was less. This trend continued so that by $\sim$780 cycles, the string was closer than ever before to its starting configuration. Clearly the recurrence had a superperiod (Fig. 2, lower). Some other force laws were computed, and in most cases they also showed a superperiod. Thus, the conjecture on equipartition also had to be dismissed. The energy ordinates in the figures derive from the Fourier coefficients $a_k[=\sum_i x_i \sin ik\pi/2N]$ according to $E_k^{\text{total}} = E_k^{\text{kinetic}} + E_k^{\text{potential}}$.
The E_k^{kinetic} comes from the velocities and is exact, but $E_k^{\text{potential}}$, as calculated from the x_i, is not: a small $\sim$ few percent error arises from neglect of the nonlinear part of the force. In one complete period of the kth mode, the energy passes from all kinetic to all potential twice. Thus the E^{total} as plotted contains a small error cyclic at twice the mode frequency. This cannot be seen on the curves, which were plotted manually, in the original FPU paper; but in Figs. 2–4, which were plotted automatically, it shows up as ripples on the energy peaks. These ripples should be regarded, therefore, at least in part, as artefacts. Since the recurrence is likely to be sensitively related to coincidence of harmonics and the like, and the number of particles used in FPU was of the form 2^P, it seemed worthwhile to check this possible source of degeneracy by making N prime; hence Fig. 3. We see that the number symmetry is not a factor. The nonlinear coefficient α determines the one-dimensional "equation of state" of the string: with α positive, we have a gas-like $\partial^2F/\partial x^2$ positive which grows shocks, for α negative, we have a physically rare $\partial^2F/\partial x^2$ negative, which grows rarefactions. Surprisingly, when the computation of Fig. 2 was run with α negative the

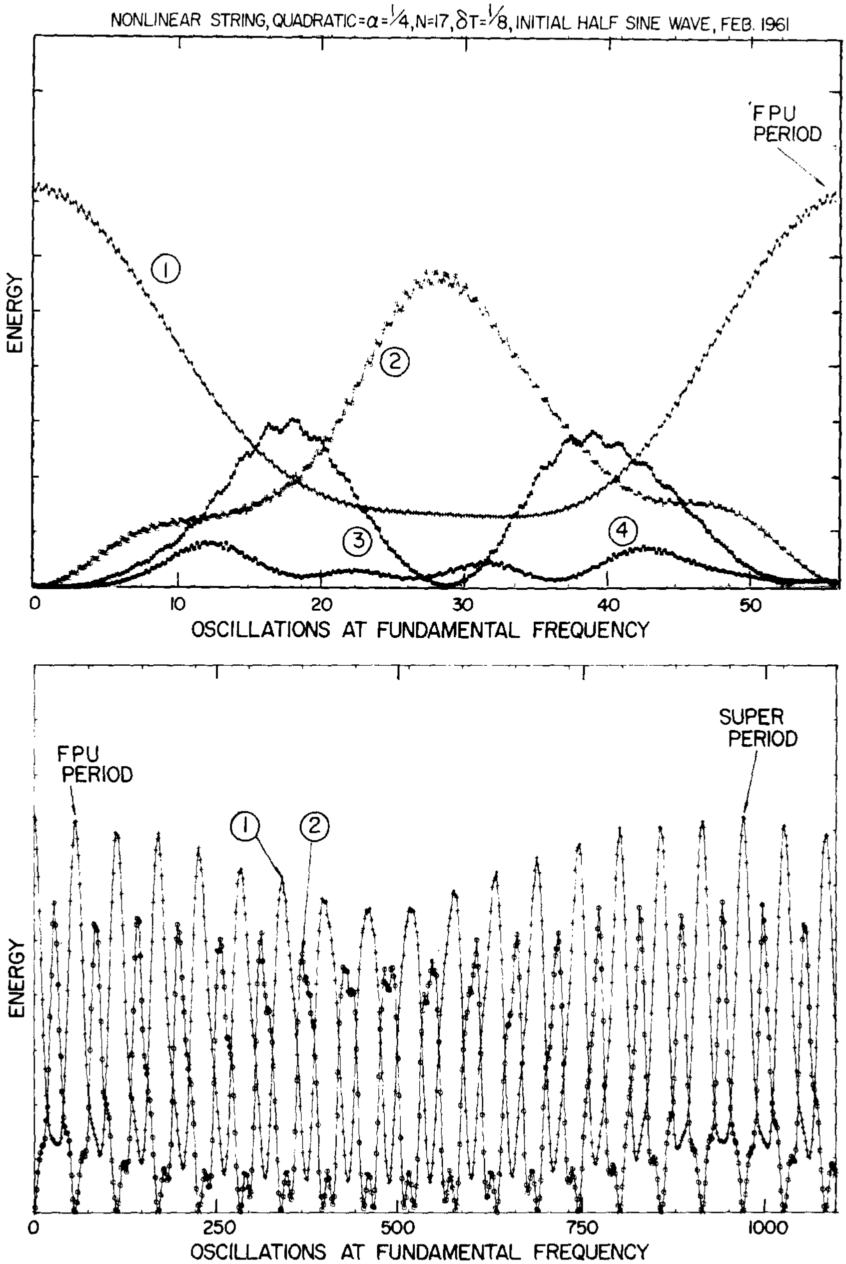

FIG. 3. As in Fig. 2, but with N increased from 16 to 17, making it prime. Qualitatively, the recurrence phenomena are unchanged. τ is increased in the ratio 17/16. Since the amplitude is unchanged, the effect of increasing N is to reduce the amount of nonlinearity, increasing τ' and τ''.

$$\begin{aligned}
\tau &= 272\,\delta t = 34 \\
\tau' &= 15{,}693\,\delta t = 196.2 = 57.69\,\tau \\
\tau'' &= 200{,}146\,\delta t = 33{,}143 = 974.8\,\tau = 16.90\,\tau'
\end{aligned}$$

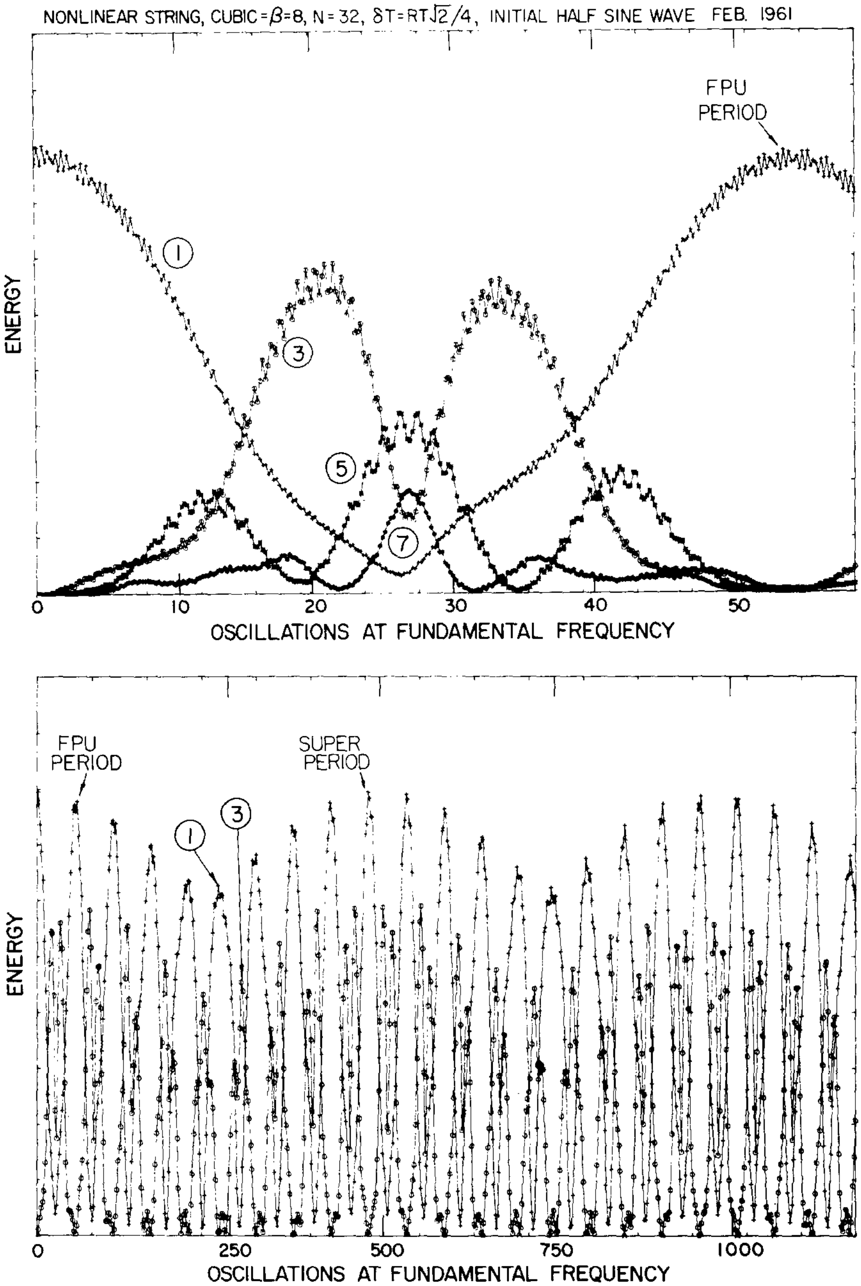

FIG. 4. As in Fig. 2 but with a cubic term $\beta = 8$, $N = 32$ and $\delta t = \sqrt{2}/4$. The cubic term maintains symmetry in the string, even modes always $= 0$.

$$\tau \qquad 181.0\,\delta t = 64$$

$$\tau' \qquad 13{,}908\,\delta t = 4916 = 76.81\,\tau$$

$$\tau'' = 121{,}110\,\delta t = 42{,}812 = 668.9\ \ \tau = 8.708\,\tau'$$

result was exactly the same. Apparently for a standing wave such as we have been studying, which is decomposable into two oppositely moving traveling waves, the differing equation of state effects cancel. But for a single wave traveling round a circular array of mass points, the steepening of sinusoids into shocks should continue. Such a computation was commenced in 1961 but was halted by an early computational instability. We are now less unfamiliar with such problems and intend to try again.

By 1961, interest in the FPU problem was stirring. A paper by Ford [5] appeared. News of the superperiod passed around. 1962–3 saw the generalization to a continuous nonlinear heavy string (Korteweg–de Vries equation) of Zabusky and Kruskal [6, 7] and the discovery of solitions. From 1966 on, distinguished contributors in countries outside the U.S. joined in. The interest in the FPU problem might be said to have reached its divergent phase. By now, the bibliography of the problem is fairly voluminous. This note is a response to requests for a superperiod reference.

Acknowledgment

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References

1. R. E. Peierls, Zur kinetischen Theorie der Warmeleitung in Kristallen, *Ann. Phys.* **3** (1929), 1055.
2. S. Chandrasekhar, Stochastic problems in physics and astronomy, *Rev. Mod. Phys.* **15** (1943), 1.
3. P. C. Hemmer, L. C. Maximon, and H. Wergeland Recurrence time of a dynamical system *Phys. Rev.* **111** (1958) 689.
4. E. Fermi, J. R. Pasta, and S. M. Ulam, "Studies of Nonlinear Problems," Los Alamos Scientific Laboratory report LA-1940 (1955); also *in* "Collected Works of Enrico Fermi," Vol. II, p. 978, University of Chicago Press, 1965.
5. J. Ford, Equipartition of energy for nonlinear systems, *J. Math. Phys.* **2** (1961), 387.
6. N. J. Zabusky, Exact solution for the vibrations of a nonlinear continuous model string, *J. Math. Phys.* **3** (1962), 1028.
7. M. D. Kruskal and N. J. Zabusky, Stroboscopic perturbation procedure for treating a class of nonlinear wave equations, *J. Math. Phys.* **5** (1964), 231.
8. P. Mazur and E. Montroll, Poincaré cycles, ergodicity, and irreversibility in assemblies of coupled harmonic oscillators, *J. Math. Phys.* **1** (1960), 70.
9. E. Teramoto, Heat flow in the linear chain of harmonically coupled particles, *Progr. Theoret. Phys. (Kyoto)* **28** (1962), 1059.

10. E. A. JACKSON, Nonlinear coupled oscillators, *J. Math. Phys.* **4** (1963), 551; **4** (1963), 686.
11. J. FORD AND J. WATERS, Computer studies of energy sharing and ergodicity for nonlinear oscillator systems, *J. Math. Phys.* **4** (1963), 1293.
12. R. S. NORTHCOTE AND R. B. POTTS, Energy sharing and equilibrium for nonlinear systems, *J. Math. Phys.* **5** (1964), 383.
13. J. WATERS AND J. FORD, A method of solution for resonant nonlinear coupled oscillator systems, *J. Math. Phys.* **7** (1966), 399.
14. F. M. ISRAELEV AND B. V. CHIRIKOV, Statistical properties of a nonlinear string, *Soviet Phys. Doklady* **11** (1966), 30.
15. B. V. CHIRIKOV, "When Does a Dynamical System Turn Into a Statistical One?," Proc. Int. Congr. Mathemat, Institute of Nuclear Physics, Moscow, 1966.
16. N. J. ZABUSKY AND G. S. DEEM, Dynamics of nonlinear lattices, *J. Computational Phys.* **2** (1967), 123.
17. N. SAITO AND H. HIROOKA, Computer studies of erogodicity in coupled oscillators with anharmonic interaction, *J. Phys. Soc. Jap.* **23** (1967), 167.
18. M. TODA, Wave propagation in anharmonic lattices, *J. Phys. Soc. Jap.* **23** (1967), 501.
19. F. M. ISRAELEV, A. I. KHISAMUTDINOV, AND B. V. CHIRIKOV, "Numerical Experiments with the Nonlinear Chain," Preprint 252, Institute of Nuclear Physics, Novosibirsk, 1968.
20. N. OOYAMA, H. HIROOKA, AND N. SAITO, Computer studies on the approach to thermal equilibrium in coupled anharmonic oscillators, II, *J. Phys. Soc. Jap.* **27** (1969), 815.
21. N. SAITO, N. OOYAMA, Y. AIZAWA, AND H. HIROOKA, Computer experiments on ergodic problems in anharmonic lattice vibrations, *Progr. Theory. Phys. (Suppl.)* 45 (1970), 209–230.
22. N. J. ZABUSKY, Nonlinear lattice dynamics and energy sharing, *J. Phys. Soc. Japan (Suppl.)* **26** (1969), 196 and references there.
23. J. FORD AND G. H. LUNSFORD, Stochastic behavior of resonant, nearly linear oscillator systems in the limit of zero nonlinear coupling, *Phys. Rev. A* **1** (1970), 59.
24. R. L. BIVINS, N. METROPOLIS, AND J. R. PASTA, "Nonlinear Coupled Oscillators: Modal Equation Approach," Los Alamos Report LA-4934, 1972.
25. E. LIEB AND D. MATTIS, "Mathematical Physics in One Dimension," Academic Press, New York, 1966.